# Orbiting Carbon Observatory-2 & -3 (OCO-2 & OCO-3)



## Solar Induced Chlorophyll Fluorescence – Data User's Guide Lite File Version 10 and VEarly

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## **Document History:**

Version	Revision	Date	Description/Comments
1.0	1	September 1, 2015	Original Document
2.0	0	September 1, 2020	Revamped document, updates for V10

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#### 1 Overview

The solar induced fluorescence (SIF) OCO-2&3 Lite files contain a subset of the information in the IMAP-DOAS (IDP) pre-processing L2 files. There is one file per day, for each day that had at least one retrieved sounding. The main purpose of the SIF-lite files is to a) perform post-processing on the original IDP files and b) provide all valid data in significantly smaller files that still contain all necessary information for typical science analyses. SIF Lite data have the some added value compared to the original IDP retrievals:

- Only contain converged soundings that passed initial quality criteria thresholds
- They include an important SIF correction procedure, performed on a daily basis using non-fluorescing surfaces such as deserts or most oceans
- They contain additional information merged from both the A Band preprocessor (ABP) as well as meteorological input data interpolated to the OCO-2&3 footprint in time and space.

The SIF-lite files are provided in <u>netCDF-4 format</u>, a self-documenting data format that allows for the organization of the data file into *Dimensions*, *Groups*, *Variables*, and *Attributes*. *Variable Attributes* provide descriptive information about each data field, including *units*, *scale\_factor*, *add\_offset*, and *description*. Figures 4-1 and 4-2 give an overview of the SIF Lite file contents. More detailed descriptions of selected fields in the SIF Lite files are given further down, but users are advised to read the *Attributes* of each *Variable* being used.

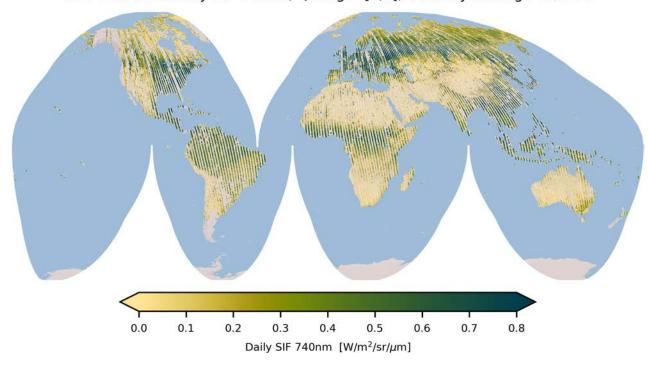
Since netCDF-4 is built on the HDF-5 storage layer, the files may be read with both netCDF4 and HDF5 software, either one generally available in most computing tools like Matlab, IDL, and Python. For Python, the use of either <a href="netCDF4">netCDF4</a> or <a href="https://document.org/h5py">h5py</a>. The <a href="Panoply Data Viewer">Panoply Data Viewer</a> is a convenient application for quickly browsing the contents of netCDF-4 files, as well as creating visualizations of the data (the SIF Lite files have not been formatted with Panoply's requirements in mind, thus your mileage may vary). Figure 4-1 shows a screenshot of the Datasets view of an OCO-3 SIF Lite file in Panoply. Older tools like <a href="https://document.org/hDFview">HDFview</a> may also still work, depending on your system.

Users of previous OCO-2 SIF Lite files (prior to Build 10) will find that the file organization has changed significantly: in addition to a set of main variables in the root group of the file, the structure of each SIF Lite file includes *Dimensions*, *Global Attributes*, and auxiliary data organized in the groups *Cloud*, *Geolocation*, *Metadata*, *Meteo*, *Offset*, and *Science*. A brief overview of the main variables and groups will be given below. It should be noted at this point that all meteorological fields in the Meteo group are taken from GEOS-5 FP-IT forecasts, and that they are provided "as is", *i.e.*, not fully validated.

Figure 1-1 shows global average Daily-Corrected SIF at 740 nm from OCO-2 and OCO-3 for June 2020, gridded to 0.20.2, which preserves the general spatial coverage of the two instruments. Figure 1-2 gives two examples of SIF at 757 nm from OCO-3 at native instrument resolution, observed in Target and Snapshot Area Map (SAM) mode.

A final note: SIF Lite files for OCO-2 and OCO-3 files have identical file structures, with information on the observing sensor provided in the *(Global) Attributes*. Furthermore, offset adjustment and quality flag assignment are performed in exactly the same way for both sensors.

OCO-2 SIF Lite: Daily SIF 740nm, QAflags=[0,1], Monthly Average 06/2020



OCO-3 SIF Lite: Daily SIF 740nm, QAflags=[0,1], Monthly Average 06/2020

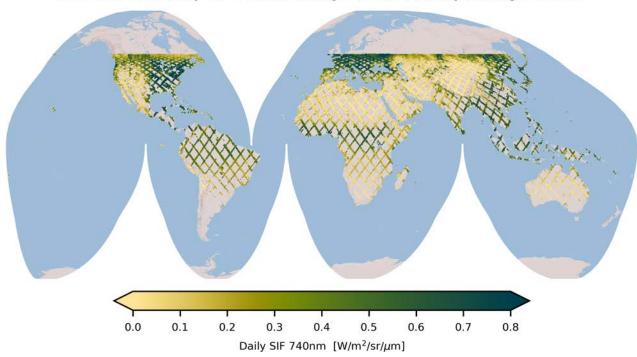


Figure 1-1: Global average Daily SIF at 740 nm from OCO-2 and OCO-3 SIF for June 2020. Data have been limited to quality flags 0 (*best*) and 1 (*good*) and gridded to 0.2°×0.2° (longitude×latitude). OCO-3 data are from the *vEarly* product.

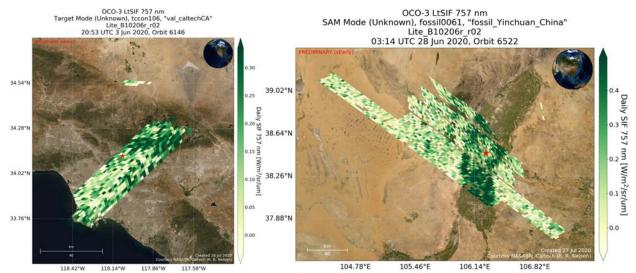


Figure 1-2: *SIF at 757 nm* observed by OCO-3 in Target Mode over Los Angeles/CalTech TCCON on 03-06-2020 (left) and in Snapshot Area Map (SAM) Mode over Yinchuan, China on 28-06-2020 (right), at native instrument resolution. OCO-3 data are from the vEarly product.

#### 2 What's New in OCO-2&3 SIF Lite V10?

#### 2.1 Data Selection

The selection of SIF soundings has changed in the current V10 version: while previously SIF data were already filtered according to basic quality criteria, the V10 SIF Lite files now include all soundings for which the standard L2 data field sounding\_qual\_flag = 0. This leads to an increase in data volume, and it also makes it necessary to filter data according to the new Quality\_Flag field (see next section).

#### 2.2 The Quality Flag

New in SIF Lite V10 is the Quality\_Flag variable that indicates the data quality level for each sounding in the OCO-2&3 SIF Lite file. Quality\_Flag is set to one of three values: best (0), good (1), and failed (2), which are assigned according to the data quality checks listed in Table 2-1. For science studies it is recommended to use the combined soundings of best&good.

```
best: Quality Flag = 0
    satisfies all of the following conditions:
         ○ 28 \le \text{continuum radiance @757 nm} \le 195 [W/m²/sr/µm]
         \circ \le \chi^2 0.757 nm \le 2.0
         \circ \leq \chi^2 \bigcirc 771 nm \leq 2.0
         \circ 0.85 \leq O<sub>2</sub> ratio \leq 1.5
         \circ 0.5 \leq CO<sub>2</sub> ratio \leq 4.0
         \circ \Theta_{sun} \leq 70^{\circ}
         Land Fraction = 100%
good: Quality_Flag = 2
    does not satisfy best but satisfies all of the following:
         ○ 28 \le \text{continuum radiance @757 nm} \le 195 [W/m<sup>2</sup>/sr/µm]
         \circ \le \chi^2 \bigcirc 757 nm \le 3.0
         ○ \leq \chi^2@771 nm \leq 3.0
         \circ 0.85 \leq O<sub>2</sub> ratio \leq 1.5
         \circ 0.5 \leq CO<sub>2</sub> ratio \leq 4.0
         \circ \Theta_{sun} \leq 70^{\circ}
         _{\circ} Land Fraction \geq 80%
failed: Quality Flag = 2
    anything neither best nor good.
```

Table 2-1: SIF Lite Quality Flag logic

Rationale for the quality screening elements:

- $\chi^2$  limits exclude fits that don't represent the spectrum well.
- continuum level radiance limits exclude scenes of high and low brightness, which might be more affected by detector calibration.
- solar zenith angle  $(\Theta_{sun})$  limit removes retrievals with large airmasses, at which rotational Raman scattering can be important.
- O<sub>2</sub> and CO<sub>2</sub> limits exclude most cloudy scenes.

It should to be noted that this quality filtering is much relaxed compared to the OCO-2&3 XCO<sub>2</sub> lite file generation, as SIF is less susceptible to atmospheric scattering. Also, unlike XCO<sub>2</sub>, SIF retrievals are accurate but imprecise, which necessitates the averaging of multiple data-points, and clouds do not strongly affect the SIF signal (Frankenberg *et al.*, 2012).

#### 2.3 Improved Bias/Offset Correction – Selection of Barren Surfaces

The SIF retrievals presented here are based on the retrieval methodologies described in Frankenberg *et al.* (2011a,b). The main retrieval quantity in the retrieval state vector is relative fluorescence, *i.e.*, the fractional contribution of SIF to the continuum level radiance. Absolute SIF is being generated in the post-processing step. Owing to various effects like uncertainties in the exact instrument line-shape per footprint or slight uncertainties in detector linearity, biases in retrieved SIF can occur. Here, we follow a similar strategy as in Frankenberg *et al.* (2011b), using reference targets to correct for biases in SIF.

The bias/offset correction requires determination of the background signal over non-fluorescing ("barren") surfaces, which is then subtracted from all SIF values. For V10, the identification of barren surfaces is based on a combination of the 2018 MODIS IGBP barren/snow land classification and Vegetation Photosynthesis Model (VPM) GPP  $\approx 0$  [Zhang *et al.*, 2017], which have been compiled into an external data base tabulated on a global grid with  $0.2^{\circ} \times 0.2^{\circ}$  resolution. The background signal is calculated from the average of SIF over barren surfaces from three days of observation (current  $\pm 1$  day).

#### 2.4 SIF at 740 nm [c.f., Parazoo *et al.*, 2019]

Satellite-based estimates of SIF are typically reported at a reference wavelength of 740 nm for moderate spectral resolution and at 757 or 771 nm for high spectral resolution sensors. This may confound intersensor comparisons. 740 nm is used because it is near the peak of the SIF emission feature in the far-red, while 757 or 771 nm as a reference wavelength for OCO-2/3 and GOSAT is driven by the ability to perform narrow band retrievals and the lack of larger spectral regions capable of performing SIF retrievals. Although the intersensor wavelength range is relatively small, absolute fluorescence values vary greatly in this region [Joiner *et al.*, 2013; Köhler *et al.*, 2018; Sun *et al.*, 2018]. Reference SIF shapes derived from leaf-level studies suggest that far-red fluorescence spectra, and thus wavelength conversions, are roughly consistent across species [Magney *et al.*, 2019].

In the OCO-2/3 V10 SIF Lite data product, the actual SIF retrievals are performed at 757 and 771 nm, and SIF at 740 nm is derived from these two balues based on the following relationship:

 $SIF@740 \text{ nm} = 1.5 \cdot (SIF@757 \text{ nm} + 2 \cdot SIF@771 \text{ nm}) / 2$ 

## 3 Specific Notes

#### 3.1 Daily Correction Factor

The Daily Correction Factor is a quantity used to estimate daily average SIF from instantaneous SIF, based on purely geometric incoming light scaling. The observed solar induced fluorescence signal is a strong function of the local illumination conditions. In the case of OCO-2, for example, the 13:30h local solar overpass time fluorescence signal particularly at high latitudes cannot be compared directly with GPP, because length-of-day and the variability of the solar zenith angle have to be taken into account. Under cloud-free conditions and ignoring Rayleigh scattering as well as gas absorption, the downwelling solar radiation scales linearly with cos(SZA). If t<sub>0</sub> denotes the time of measurement in fractional days, a first order approximation for a daily fluorescence average can be written as:

$$\overline{F}_{S} = F_{S} / \cos(SZA(t_{0})) \cdot \int_{t=t_{0}-12h}^{t=t_{0}+12h} \cos(SZA(t))dt$$

The correction  $\cos(SZA(t_0)) \cdot \int_{t-t_0-12h}^{t=t_0+12h} \cos(SZA(T)) dt$  is computed with the integral sampled numerically in 10 minute time-steps (Python's <u>pyEphem</u> package), and reported in the SIF Lite file at is provided in /Science/daily\_correction\_factor for each sounding as a function of latitude, longitude and time.

#### 3.2 What (Not) To Do With Negative Values

In a nutshell: Do not discard negative SIF values outright! It is important to note that the 1- $\sigma$  uncertainties of all SIF values can be substantial, which can can lead to negative SIF values. Owing to the presence of retrieval noise, negative values are perfectly valid in a measurement retrieval sense, and discarding them will introduce a bias in any averages that are being computed. In general, multiple soundings will need to be averaged to reduce the noise by a factor of  $1/\sqrt{n}$ , with n being the number of averages.

That being said, extreme negative values can indicate a problem during the retrieval. Thus, it is recommended to accept/reject negative SIF values based on the following considerations:

- SIF + 2- $\sigma$  Uncertainty >= 0: sounding is valid; accept.
- SIF + 2- $\sigma$  Uncertainty < 0 but SIF + 3- $\sigma$  Uncertainty >= 0: sounding quality is questionable; accept or reject.
- SIF +  $3-\sigma$  Uncertainty < 0: retrieved SIF is most likely invalid; reject.

The SIF Lite post-processing currently does not check for these conditions when assigning the quality flag, though this may be implemented in future releases.

#### 4 File Structure & Fields

The primary variables that most users will be interested in are located in the root level (/) of the SIF Lite file. Some of these variables are duplicated in the Science group. Auxiliary data fields are organized in groups, according to either their orgin (*Cloud, Meteo*) or their nature (*Geolocation, Metadata, Offset, Science*). Figure 4-1 below shows a partial view of an OCO-3 SIF Lite file using the <u>Panoply Data Viewer</u>, and Figure 4-2 lists all variables, groups, and global attributes.

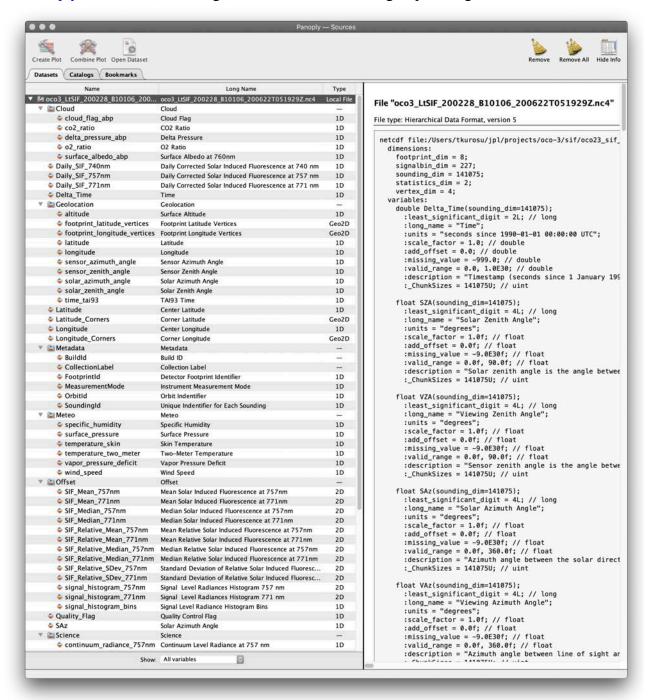


Figure 4-1: Panoply Datasets view (partial) of an OCO-3 SIF Lite file.

```
netcdf oco3_LtSIF_200609_B10206r_200713163557s
dimensions:
     footprint_dim;
                            signalbin_dim;
                                               sounding_dim;
                                                                   statistics_dim;
                                                                                      vertex_dim;
global attributes:
    References;
                            conventions:
                                                         product version:
                                                                                      summarv:
    keywords;
                            keywords_vocabulary;
                                                         .
cdm_data;
                                                                                      comment:
    date_created;
                            author_name;
                                                         author_email;
                                                                                      secondary_author_name;
    secondary_author_email; project;
                                                         geospatial_lat_min;
                                                                                      geospatial_lat_max;
     geospatial_lat_units; geospatial_lon_min;
                                                         geospatial_lon_max;
                                                                                      geospatial_lon_units;
                                                         spatial_resolution;
     platform;
                            sensor;
                                                                                      date_time_coverage;
     day_of_year_coverage; InputCollectionLabel;
                                                         InputBuildId;
                                                                                      InputPointers;
    CoordSysBuilder;
                            identifier_product_doi;
                                                         identifier_product_doi_authority;
variables:
    double Delta_Time(sounding_dim);
    float SZA(sounding_dim);
                                                         float VZA(sounding_dim);
     float SAz(sounding_dim);
                                                         float VAz(sounding_dim);
     float Longitude(sounding_dim);
                                                         float Latitude(sounding_dim);
     float Longitude_Corners(sounding_dim, vertex_dim); float Latitude_Corners(sounding_dim, vertex_dim);
     float SIF_740nm(sounding_dim);
                                                         float SIF_Uncertainty_740nm(sounding_dim);
     float Daily SIF 740nm(sounding dim);
                                                         float Daily SIF 757nm(sounding dim);
     float Daily_SIF_771nm(sounding_dim);
                                                         short Quality_Flag(sounding_dim);
group: Cloud
  variables:
     float surface_albedo_abp(sounding_dim);
                                                         short cloud_flag_abp(sounding_dim);
     float delta_pressure_abp(sounding_dim);
                                                         float co2_ratio(sounding_dim);
    float o2_ratio(sounding_dim);
group: Geolocation
  variables:
     double time_tai93(sounding_dim);
                                                float solar_zenith_angle(sounding_dim);
     float solar_azimuth_angle(sounding_dim); float sensor_zenith_angle(sounding_dim);
     float sensor_azimuth_angle(sounding_dim); float altitude(sounding_dim);
     float longitude(sounding_dim);
                                               float footprint_longitude_vertices(sounding_dim, vertex_dim);
     float latitude(sounding_dim);
                                               float footprint_latitude_vertices(sounding_dim, vertex_dim);
group: Metadata
  variables:
                                      string BuildId int OrbitId(sounding dim);
     string CollectionLabel;
                                                                                      int64
     SoundingId(sounding_dim);
    int64 FootprintId(sounding_dim); short MeasurementMode(sounding_dim);
  variables:
    float surface_pressure(sounding_dim);
                                                         float specific_humidity(sounding_dim);
    float vapor_pressure_deficit(sounding_dim);
                                                         float temperature_skin(sounding_dim);
    float temperature_two_meter(sounding_dim);
                                                         float wind_speed(sounding_dim);
group: Offset
  variables:
     float signal_histogram_bins(signalbin_dim);
     int signal_histogram_757nm(signalbin_dim, footprint_dim);
     int signal_histogram_771nm(signalbin_dim, footprint_dim);
     float SIF_Relative_Mean_757nm(signalbin_dim, footprint_dim, statistics_dim);
    float SIF_Mean_757nm(signalbin_dim, footprint_dim, statistics_dim);
    float SIF_Relative_Median_757nm(signalbin_dim, footprint_dim, statistics_dim);
float SIF_Median_757nm(signalbin_dim, footprint_dim, statistics_dim);
     float SIF_Relative_SDev_757nm(signalbin_dim, footprint_dim, statistics_dim);
     float SIF_Relative_Mean_771nm(signalbin_dim, footprint_dim, statistics_dim);
     float SIF_Mean_771nm(signalbin_dim, footprint_dim, statistics_dim);
     float SIF_Relative_Median_771nm(signalbin_dim, footprint_dim, statistics_dim);
     float SIF_Median_771nm(signalbin_dim, footprint_dim, statistics_dim);
     float SIF Relative SDev 771nm(signalbin dim, footprint dim, statistics dim);
group: Science
  variables:
     short sounding_qual_flag(sounding_dim);
                                                                   short IGBP_index(sounding_dim);
     float continuum_radiance_757nm(sounding_dim);
                                                                   float SIF_757nm(sounding_dim);
     float SIF_Unadjusted_757nm(sounding_dim);
                                                                   float SIF_Relative_757nm(sounding_dim);
     float SIF_Unadjusted_Relative_757nm(sounding_dim);
                                                                   float SIF_Uncertainty_757nm(sounding_dim);
     float continuum_radiance_771nm(sounding_dim);
                                                                   float SIF_771nm(sounding_dim);
     float SIF Unadjusted 771nm(sounding dim);
                                                                   float SIF Relative 771nm(sounding dim);
     float SIF_Unadjusted_Relative_771nm(sounding_dim);
                                                                   float SIF_Uncertainty_771nm(sounding_dim);
float daily_correction_factor(sounding_dim);
                                                         float sounding_land_fraction(sounding_dim);
```

Figure 4-2: ncdump overview of the contents of an OCO-2&3 SIF Lite file.

#### 4.1 Dimensions

Table 4-1 lists the five dimensions that define all the array variables in the SIF Lite file. only sounding\_dim, the number of observations, is variable; all others are fixed.

Table 4-1: Array Dimensions.

Dimension	Description	
sounding_dim (variable)	Number of soundings (observations) in the file.	
footprint_dim (8)	Number of OCO-2&3 across-track footprints	
vertex_dim (4)	Number of footprint corner co-ordinates	
signalbin_dim (227)	Number of entries in the signal histogram arrays (/Offset group)	
statistics_dim (2)	Array dimension in the Mean and Median SIF values (/Offset group), representing adjusted and unadjusted values	

#### 4.2 Global Attributes

Table 4-2 lists the names of all *Global Attributes* in the file. *Global Attributes* help with book-keeping and source identification, and can safely be ignored for standard applications. However, some of the attributes may be helpful for advanced applications or recovering information on temporal coverage, *e.g.*, in cases where file names have been lost. Table 2.2 summarizes a few of the Global Attributes that might be most helpful.

Table 4-2: Selected Global Attributes.

Attribute	Description	
date_time_coverage	UTC time string of first and last observation in the file. Example: "2020-02-28T01:18:41.896032Z", "2020-02-28T23:00:10.977032Z"	
day_of_year_coverage	Similar to date_time_coverage, but with day-of-year instead of year-month-day. Example "2020-059T01:18:41.896032Z", "2020-059T23:00:10.977032Z"	
InputCollectionLabel	Collection Label of the L2 data products used in the creation of the SIF Lite file. Example: "SCF_B10110_r01"	
InputBuildId	Build ID of the L2 data products used in the creation of the SIF Lite file. Example: "B10.1.06"	
InputPointers	String with the names of all input products and auxiliary data used in the creation of the SIF Lite file. Note that the calculation of the offset adjustment is performed using a three-day window (current day±1), so this string tends to be long.	

#### 4.3 Root Level (/) Variables

Table 4-3 summarizes the data fields in the root level of the file, *i.e.*, the variables that are likely to be of main interest to most users. Variables related to latitude, longitude, and observation geometry are duplicated in the /Geolocation group. Daily\_SIF variables have been corrected for length-of-day illumination (see section 3.1).

Table 4-3: Root Level Variables

Attribute	Units	Description
Daily_SIF_757 nm	W/m²/sr/µm	Daily Corrected Solar Induced Fluorescence at 757 nm. Daily_SIF_757 nm = /Science/sif_757 nm * /Science/daily_correction_factor
Daily_SIF_771 nm	W/m²/sr/µm	Daily Corrected Solar Induced Fluorescence at 771 nm; typically about 1.5 times smaller value than at 757 nm.  Daily_SIF_771 nm = /Science/sif_771 nm * /Science/daily_correction_factor
Daily_SIF_740 nm	W/m²/sr/µm	Daily Corrected Solar induced chlorophyll fluorescence at 740 nm.  Daily_SIF_740 nm = SIF_740 * /Science/daily_correction_factor
SIF_740 nm	W/m²/sr/µm	Solar Induced Fluorescence at 740 nm. SIF at retrieved wavelength: SIF_740 nm = 0.75 * (/Science/sif_757 nm + 1.5*/Science/sif_771 nm)
SIF_Uncertainty_740 nm	W/m²/sr/µm	Estimated 1-Sigma Uncertainty of Solar Induced Fluorescence at 740 nm. Uncertainty computed from continuum level radiance at 740 nm: SIF_Uncertainty_740 = 0.75*((/Science/sif_757 nm)² + (1.5*/Science/sif_771 nm)²)½.
Quality_Flag	N/A	Quality Control Flag. SIF Lite Quality Flag: 0 = best (passes quality control + cloud fraction = 0.0); 1 = good (passes quality control); 2 = bad (failed quality control); -1 = not investigated.
Latitude	°N (Degrees North)	Footprint Center Latitudes. Center latitudes of the measurement ground pixel.
Latitude_Corners	°N	Footprint Corner Latitudes. Corner latitudes of the measurement ground pixel.
Longitude	°E	Footprint Center Longitudes. Center longitudes of the measurement ground pixel.
Longitude_Corners	°E	Footprint Corner Longitudes. Corner longitudes of the measurement ground pixel.
Delta_Time	seconds	Timestamp. Elapsed seconds since 1990-01-01 00:00:00 UTC.
SZA	٥	Solar Zenith Angle. Zenith the angle between the line of sight to the sun and the local vertical.
SAz	0	Solar Azimuth Angle. Azimuth angle between the solar direction as defined by the sounding location, and the sounding local North.
VZA	0	Viewing Zenith Angle. Zenith angle between sensor line-of-sight and local vertical.
VAz °		Viewing Azimuth Angle. Azimuth angle between sensor line-of-sight and local North.

## 4.4 The Cloud Group

The /Cloud group contains a select number of variables from the L2ABP product, related to clouds and surface albedo. /Cloud/co2\_ratio and /Cloud/o2\_ratio are used in the assignment of the Quality Flag. Variable are summarized in Table 4-4.

Table 4-4: Cloud Group Variables

Attribute	Units	Description
cloud_flag_abp	N/A	Indicator of whether the sounding contained clouds: 0="Classified clear", 1="Classified cloudy", 2="Not classified", all other values undefined; not used in SIF Lite processing.
co2_ratio	N/A	Ratio of CO <sub>2</sub> retrieved in weak and strong CO <sub>2</sub> band (value near 1 indicate scattering free scene).
delta_pressure_abp	Pa	Retrieved-predicted surface pressure from ABO2, usable as cloud screener; not used in SIF Lite processing.
o2_ratio	N/A	Ratio of retrieved and predicted O <sub>2</sub> column in the 771 nm window. Data quality of <i>good</i> and <i>best</i> require values between 0.85 and 1.5.
surface_albedo_abp	N/A	Surface albedo (lambertian equivalent) as retrieved in the ABO2 preprocessor at 760 nm; not used in SIF Lite processing.

#### 4.5 The Geolocation Group

The /Geolocation group collects variables related to footprint latitude, longitude, viewing geometry, altitude, and the TAI93 time stamp. It duplicates several of the Root Level variables, albeit with different data field names, because the convenience of collecting all geolocation-related variables in one group is considered worth the small increase of file size the duplicate fields create.

Table 4-5: Geolocation Group Variables

Attribute	Units	ts Description	
altitude	meters	Surface altitude [m] of observed footprint.	
footprint_latitude_vertices	°N	Footprint Corner Latitudes [Degrees North]. Corner latitudes of the measurement ground pixel. <i>cf.</i> , /Latitude_Corners	
footprint_latitude_vertices	°E	Footprint Corner Longitudes [Degrees East]. Corner longitudes of the measurement ground pixel. <i>cf.</i> , /Longitude_Corners	
latitude	°N	Footprint Center Latitudes [Degrees North]. Center latitudes of the measurement ground pixel. <i>cf.</i> , /Latitude	
Longitude	°E	Footprint Center Longitudes [Degrees East]. Center longitudes of the measurement ground pixel. <i>cf.</i> , /Longitude	
sensor_azimuth_angle	degrees	Sensor Azimuth Angle [Degrees]. Azimuth angle between sensor line-of-sight and local North. cf., NAz	
sensor_zenith_angle	degrees	Viewing Zenith Angle [Degrees]. Zenith angle between sensor line-of-sight and local vertical.	
solar_azimuth_angle	degrees	Solar Azimuth Angle [Degrees]. Azimuth angle between the solar direction as defined by the sounding location, and the sounding local North. cf., /SAz	
solar_zenith_angle	degrees	Solar Zenith Angle [Degrees]. Zenith the angle between the line of sight to the sun and the local vertical. cf., /SZA	
time_tai93	seconds	Timestamp [seconds]. Elapsed seconds since 1993-01-01 00:00:00 UTC.	

## 4.6 The Metadata Group

Variables in the /Metadata group (Table 4-6) collect information on the ground footprints that is useful for separating observation modes (e.g., nadir, glint, target, area map, etc.) and when comparing footprints values between different product files.

Table 4-6: Metadata Group Variables

Attribute	Description	
Footprintld	OCO-2 or OCO-3 footprint identifier (1-8), identifying the 8 independent cross-track spatial samples per frame.	
MeasurementMode	Instrument Measurement Mode, 0=Nadir, 1=Glint, 2=Target, 3=AreaMap*, 4=Transition*; users might consider to separate these for analysis. *OCO-3 only.	
Orbitld	Orbit Identifier: Start Orbit Number (OCO-2) or Start Solar Day (OCO-3) of observation.	
SoundingId	Unique Identifier for each sounding, consistent across all products. Use this identifier when matching footprints between OCO-2 or OCO-3 product files. Format: YYYYMMDDHHMMSS.	

## 4.7 The Meteo Group

The /Meteo group collects meteorological forecast quantities, taken from the GEOS-5 FP-IT model. See Table 4-7.

Table 4-7: Meteo Group Variables.

Attribute	Units	Description
specific_humidity	kg/kg	Specific humidity at surface layer at the sounding location, interpolated from GEOS-5 FP-IT inst3_3d_asm_Nv field QV (specific_humidity).
		Surface pressure at the sounding location; interpolated from GEOS-5 FP-IT inst3_3d_asm_Nv field PS (surface_pressure).
temperature_skin	К	Skin temperature at the sounding location; interpolated from GEOS-5 FP-IT inst3_2d_asm_Nx field TS (surface_skin_temperature).
temperature_two_meter	К	Two-meter temperature at the sounding location; interpolated from GEOS-5 FP-IT inst3_2d_asm_Nx field T2M (2-meter_air_temperature).
vapor_pressure_deficit Pa		Vapor pressure deficit at the sounding location (2m).
wind_speed	m/sec	Surface wind speed at sounding location; interpolated from GEOS-5 FP-IT inst3_2d_asm_Nx field U10M and inst3_2d_asm_Nx field V10M (10-meter_eastward_wind, 10-meter_northward_wind).

## 4.8 The Offset Group

The /Offset group (Table 4-8) collects variables with information on statistics of the offset/bias adjustment: mean, median, and standard deviations of original ("unadjusted") and bias-adjusted SIF values at 757 nm and 771 nm, separated by cross-track footprint. All data are are reported on a grid of signal level bins with range 3.0 to 229.0  $W/m^2/sr/\mu m$ .

Table 4-8: Offset Group Variables.

Attribute	Units	Description
SIF_Mean_757 nm	W/m²/sr/µm	Specific humidity at surface layer at the sounding location, interpolated from GEOS-5 FP-IT inst3_3d_asm_Nv field QV (specific_humidity).
SIF_Mean_771 nm	W/m²/sr/µm	Surface pressure at the sounding location; interpolated from GEOS-5 FP-IT inst3_3d_asm_Nv field PS (surface_pressure).
SIF_Median_757 nm	W/m²/sr/µm	Skin temperature at the sounding location; interpolated from GEOS-5 FP-IT inst3_2d_asm_Nx field TS (surface_skin_temperature).
SIF_Median_771 nm	W/m²/sr/µm	Two-meter temperature at the sounding location; interpolated from GEOS-5 FP-IT inst3_2d_asm_Nx field T2M (2-meter_air_temperature).
SIF_Relative_Mean_757 nm	N/A	Vapor pressure deficit at the sounding location (2m).
SIF_Relative_Mean_771 nm	N/A	Surface wind speed at sounding location; interpolated from GEOS-5 FP-IT inst3_2d_asm_Nx field U10M and inst3_2d_asm_Nx field V10M (10-meter_eastward_wind, 10-meter_northward_wind).
SIF_Relative_Median_757 nm	N/A	Mean relative Solar Induced Fluorescence at 757 nm (by footprint, for adjusted and unadjusted values).
SIF_Relative_Median_771 nm	N/A	Mean relative Solar Induced Fluorescence at 771 nm (by footprint, for adjusted and unadjusted values).
SIF_Relative_SDev_757 nm	N/A	Standard deviation of relative Solar Induced Fluorescence at 757 nm (by footprint, for adjusted and unadjusted values).
SIF_Relative_SDev_771 nm	N/A	Standard deviation of relative Solar Induced Fluorescence at 771 nm (by footprint, for adjusted and unadjusted values).
signal_histogram_757 nm	N/A	Signal level histogram for 757 nm radiances.
signal_histogram_771 nm	N/A	Signal level histogram for 771 nm radiances.
signal_histogram_bins	W/m <sup>2</sup> /sr/µm	Radiance level offset histogram bins.

## 4.9 The Science Group

Table 4-9 lists all entries in the /Science group. This group contains SIF values at 757 nm and 771 nm in various aspects: offset-adjusted for background and original values, both absolute numbers and relative to the continuum level radiances, and the  $1-\sigma$  uncertainties for SIF at both wavelengths. This group also includes the daily correction factor for local illumination, and the land fraction for each ground footprint. IGBP index is included, even though this quantity is no longer used in the identification of barren SIF surfaces.

Table 4-9: Science Group Variables.

Attribute	Units	Description
continuum_radiance_757 nm	W/m²/sr/µm	Continuum Level Radiance at 757 nm. OCO-2&3 radiances are multiplied by a factor 2 to account for unpolarized light.
continuum_radiance_771 nm	W/m²/sr/µm	Continuum Level Radiance at 771 nm. OCO-2&3 radiances are multiplied by a factor 2 to account for unpolarized light.
daily_correction_factor	N/A	Correction factor to estimate daily average SIF from instantaenous SIF (using pure geometric incoming light scaling).
IGBP_index	N/A	IGBP One-Minute Land Ecosystem Classification Product is a global (static map) data set of the International Geosphere-Biosphere Programme (IGBP) classification scheme stored on an equal-angle rectangular grid at 1-minute resolution. No longer used in SIF Lite processing.
SIF_757 nm	W/m²/sr/µm	Offset-Adjusted Solar Induced Chlorophyll Fluorescence at 757 nm.
SIF_771 nm	W/m²/sr/µm	Offset-Adjusted Solar Induced Chlorophyll Fluorescence at 771 nm; typically about 1.5 times smaller value than at 757 nm.
SIF_Relative_757 nm	N/A	Solar Induced Chlorophyll Fluorescence at 757 nm, no offset adjustment.
SIF_Relative_771 nm	N/A	Offset-Adjusted Solar Induced Chlorophyll Fluorescence at 771 nm in fractions of continuum level.
SIF_Unadjusted_757 nm	W/m²/sr/µm	Solar Induced Chlorophyll Fluorescence at 757 nm, no offset adjustment.
SIF_Unadjusted_771 nm	W/m²/sr/µm	Solar Induced Chlorophyll Fluorescence at 771 nm, no offset adjustment.
SIF_Unadjusted_Relative_757 nm	N/A	Solar Induced Chlorophyll Fluorescence at 757 nm in fractions of continuum level, no offset adjustment.
SIF_Unadjusted_Relative_771 nm	N/A	Solar Induced Chlorophyll Fluorescence at 771 nm in fractions of continuum level, no offset adjustment.
SIF_Uncertainty_757 nm	W/m²/sr/µm	One-Sigma Statistical Uncertainty in Solar Induced Chlorophyll Fluorescence at 757 nm.
SIF_Uncertainty_771 nm	W/m²/sr/µm	One-Sigma Statistical Uncertainty in Solar Induced Chlorophyll Fluorescence at 771 nm.
sounding_land_fraction	%	Percentage of land surface type within the sounding.
sounding_qual_flag	N/A	Sounding Quality Flag: 0 = good, 1 = bad.

#### 5 References

- Frankenberg, C., Butz, A., & Toon, G. C. (2011a). Disentangling chlorophyll fluorescence from atmospheric scattering effects in O2 A-band spectra of reflected sun-light. Geophysical Research Letters, 38, L03801.
- Frankenberg, C., Fisher, J., Worden, J., Badgley, G., Saatchi, S., Lee, J.-E., et al. (2011b). New global observations of the terrestrial carbon cycle from GOSAT: Patterns of plant fluorescence with gross primary productivity. Geophysical Research Letters, 38(17), L17706.
- Frankenberg, C., O'Dell, C., Guanter, L., & McDuffie, J. (2012). Remote sensing of near-infrared chlorophyll fluorescence from space in scattering atmospheres: implications for its retrieval and interferences with atmospheric CO2 retrievals. Atmospheric Measurement Techniques, 5(8), 20812094.
- Frankenberg, C., O'Dell, C., Berry, J., Guanter, L., Joiner, J., Khler, P., et al. (2014). Prospects for chlorophyll fluorescence remote sensing from the Orbiting Carbon Observatory-2. Remote Sensing of Environment, 147(0), 112.
- Guanter, L., Rossini, M., Colombo, R., Meroni, M., Frankenberg, C., Lee, J.-E., & Joiner, J. (2013). Using field spectroscopy to assess the potential of statistical approaches for the retrieval of sun-induced chlorophyll fluorescence from ground and space. Remote Sensing of Environment, 133(0), 5261.
- Guanter, L., Frankenberg, C., Dudhia, A., Lewis, P. E., Gómez-Dans, J., Kuze, A., et al. (2012). Retrieval and global assessment of terrestrial chlorophyll fluorescence from GOSAT space measurements. Remote Sensing of Environment, 121, 236251.
- Joiner, J., Guanter, L., Lindstrot, R., Voigt, M., Vasilkov, A. P., Middleton, E. M., et al. (2013). Global monitoring of terrestrial chlorophyll fluorescence from moderate spectral resolution near-infrared satellite measurements: Methodology, simulations, and application to GOME-2. Atmospheric Measurement Techniques Discussions, 6(2), 3883–3930. <a href="https://doi.org/10.5194/amtd-6-3883-2013">https://doi.org/10.5194/amtd-6-3883-2013</a>.
- Köhler, P., Guanter, L., Kobayashi, H., Walther, S., & Yang, W. (2018). Assessing the potential of Sun-induced fluorescence and the canopy scattering coefficient to track large-scale vegetation dynamics in Amazon forests. Remote Sensing of Environment, 204, 769–785. https://doi.org/10.1016/j.rse.2017.09.025
- Lee, J.-E., Frankenberg, C., van der Tol, C., Berry, J. A., Guanter, L., Boyce, C. K., et al. (2013). Forest productivity and water stress in Amazonia: observations from GOSAT chlorophyll fluorescence. Proceedings of the Royal Society B: Biological Sciences, 280(1761).
- Magney, T. S., Frankenberg, C., Khler, P., North, G., Davis, T. S., Dold, C., et al. (2019). Disentangling changes in the spectral shape of chlorophyll fluorescence: implications for remote sensing of photosynthesis. Journal of Geophysical Research: Biogeosciences, 124, 1491–1507. https://doi.org/10.1029/2019JG005029

- Parazoo, N.C., C. Frankenberg, P. Kohler, J. Joiner, Y. Yoshida, T. Magney, Y. Sun, V. Yadav, Towards a harmonized long-term spaceborne record of far-red solar induced fluorescence, 2019: JGR-Biogeosciences, 124 (8), 2518-2539.
- Sun, Y., Frankenberg, C., Jung, M., Joiner, J., Guanter, L., Köhler, P., & Magney, T. (2018). Overview of solar-induced chlorophyll fluorescence (SIF) from the Orbiting Carbon Observatory-2: Retrieval, cross-mission comparison, and global monitoring for GPP. Remote Sensing of Environment, 209(February), 808–823. https://doi.org/10.1016/j.rse.2018.02.016
- Zhang, Y., Xiao, X., Wu, X. *et al.* A global moderate resolution dataset of gross primary production of vegetation for 2000–2016. *Sci Data* **4**, 170165 (2017). <a href="https://doi.org/10.1038/sdata.2017.165">https://doi.org/10.1038/sdata.2017.165</a>.